

Pentadecanal-

Other names:	1-Pentadecanal n-Pentadecanal
Inchi:	InChI=1S/C15H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h15H,2-14H2,1H3
InchiKey:	XGQJZNCFDLXSIJ-UHFFFAOYSA-N
Formula:	C15H30O
SMILES:	CCCCCCCCCCCCCCC=O
Mol. weight [g/mol]:	226.40
CAS:	2765-11-9

Physical Properties

Property code	Value	Unit	Source
gf	-24.10	kJ/mol	Joback Method
hf	-438.51	kJ/mol	Joback Method
hfus	36.90	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.277		Crippen Method
mcpvol	223.780	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	1713.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1707.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1693.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1690.00		NIST Webbook
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rinpol	1713.00		NIST Webbook
rinpol	1719.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2024.00		NIST Webbook
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ripol	2012.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	2041.00		NIST Webbook
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ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
tb	559.15 ± 4.00	K	NIST Webbook
tc	755.45	K	Joback Method
tf	297.70 ± 3.00	K	NIST Webbook
tf	298.00 ± 4.00	K	NIST Webbook
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.03	J/mol×K	591.26	Joback Method
cpg	607.40	J/mol×K	618.63	Joback Method
cpg	624.05	J/mol×K	645.99	Joback Method
cpg	640.01	J/mol×K	673.36	Joback Method
cpg	655.29	J/mol×K	700.72	Joback Method
cpg	669.91	J/mol×K	728.09	Joback Method
cpg	683.90	J/mol×K	755.45	Joback Method
dvisc	0.0043788	Pa×s	300.81	Joback Method
dvisc	0.0018114	Pa×s	349.22	Joback Method
dvisc	0.0009290	Pa×s	397.63	Joback Method
dvisc	0.0005507	Pa×s	446.03	Joback Method
dvisc	0.0003617	Pa×s	494.44	Joback Method
dvisc	0.0002560	Pa×s	542.85	Joback Method
dvisc	0.0001918	Pa×s	591.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2765119&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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